

Heptanedioic acid
111-16-0 | DTXSID5021598

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.72	51.8	0.74	50.3	0.73	52.7

Model Results

Predicted value: 110 °C

Global applicability domain: Inside

Local applicability domain index: 8.50e-01

Confidence level: 5.77e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>Heptanedioic acid</div> <div>Measured: 106</div> <div>Predicted: 110</div>	<div>Image not found</div> <div>Octanedioic acid</div> <div>Measured: 144</div> <div>Predicted: 115</div>	<div>Image not found</div> <div>3-Methylglutaric acid</div> <div>Measured: 87.0</div> <div>Predicted: 110</div>
<div>Image not found</div> <div>2-METHYLHEXANEDIOIC ACID</div> <div>Measured: 64.0</div> <div>Predicted: 90.6</div>	<div>Image not found</div> <div>Hexanedioic acid</div> <div>Measured: 153</div> <div>Predicted: 124</div>	